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Solving The Long-Standing Problem Of Nuclear Reactions At The Highest Microscopic Level: Annual Continuation And Progress Report

S. Quaglioni

March 11, 2014

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

March 5, 2014 LLNL-TR-651616

DOE OFFICE OF SCIENCE
OFFICE OF NUCLEAR PHYSICS
NUCLEAR THEORY DIVISION

DOE National Laboratory Announcement LAB 10-395

SOLVING THE LONG-STANDING PROBLEM OF LOW-ENERGY NUCLEAR REACTIONS AT THE HIGHEST MICROSCOPIC LEVEL

ANNUAL CONTINUATION AND PROGRESS REPORT

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Work Proposal Number: SCW1158
Budget & Reporting code: KB0301020
Project Period: June 14, 2011 – June 13, 2016
Reporting Period: Year-3, August 15, 2013 – August 14, 2014
Reporting Frequency: Annual

Auspices
Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

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Background

The project "Solving the Long-Standing Problem of Low-Energy Nuclear Reactions at the Highest Microscopic Level" is an Early Career Research Program (ECRP) project funded by the Nuclear Theory Division of the Office of Nuclear Physics. Funding for this project was approved in June 2011, and became available to the PI at the beginning of August 2011. Therefore, the reporting period for Year 3 of the present project is August 15, 2013 – August 14, 2014. The present Continuation and Progress report is based on the first 7 months (August 15, 2013 – March 14, 2014) of such reporting period. The funding supports, each year, the Principal Investigator (Sofia Quaglioni), one Postdoctoral Researcher, and one Ph.D. student hired for three months during the summer. The Postdoctoral Researcher for the review period (Guillaume Hupin) was hired in December 2012 and will be employed until end of July 2014. We are currently in the process of identifying a new Postdoctoral Researcher. Micah Schuster, San Diego State University, is the Ph.D. student for the period under review.

Objectives

The aim of this project is to develop a comprehensive framework that will lead to a fundamental description of both structural properties and reactions of light nuclei in terms of constituent protons and neutrons interacting through nucleon-nucleon (*NN*) and three-nucleon (*NNN*) forces. This project will provide the research community with the theoretical and computational tools that will enable: (1) an accurate prediction for fusion reactions that power stars and Earth-based fusion facilities; (2) an improved description of the spectroscopy of exotic nuclei, including light Borromean systems; and (3) a fundamental understanding of the three-nucleon force in nuclear reactions and nuclei at the drip line.

To achieve this goal, we build upon a promising technique emerged recently as a candidate to reach a fundamental description of low-energy binary reactions between light ions, that is the *ab initio* no-core shell model combined with the resonating-group method (NCSM/RGM).[1,2] This approach has demonstrated the capability to describe binary reactions below the three-body breakup threshold[3,4] based, up to now, on similarity-renormalization-group (SRG)[5] evolved *NN* only potentials. To advance the understanding of nuclear reactions at low energies and light exotic nuclei, this project aims at extending the NCSM/RGM approach to include the full range of *NNN* interactions as well as the treatment of three-cluster bound and continuum states. Three-nucleon interactions are unavoidable components of a fundamental nuclear Hamiltonian obtained in a low-energy effective theory. In addition, three-nucleon force terms are induced by the SRG procedure and have to be taken into account for such a transformation to be unitary in many-body calculations. At the same time, the introduction of three-body cluster states is key to achieve a microscopic description of Borromean systems as well as three-body breakup reactions. This project will both enhance the fundamentality and enlarge the scope of our microscopic description of nuclear properties.

A successful completion of this project will result in improved accuracy of the ^{3}He(^{3}He,2p)^{4}He and ^{3}He(α,γ)^{7}Be reaction rates and consequently, in enhancement of the predictive capability of the standard solar model. In addition, we will study also the mirror reactions ^{3}H(^{3}H,2n)^{4}He and $^{3}H(\alpha,\gamma)^{7}Li$ (a key reaction for the production of ^{7}Li in the standard big-bang nucleosynthesis), and the spectroscopy of the ^{6}He, ^{6}Be, and ^{11}Li nuclei.

Accomplishments

Major Goals and Objectives for the Review Period

Extending the *ab initio* NCSM/RGM approach to include *NNN* forces and three-cluster nuclear states in the continuum is mathematically and computationally non-trivial, requiring several development stages. Therefore, we plan to develop these two extensions gradually, at first separately, mindful that a fully converged calculation of a reaction like the ^{3}He(^{3}He,2*p*)^{4}He fusion, including the *NNN* force, might require the deployment of exaflop machines. This strategy will allow us to perform important intermediate applications, while setting up all needed components of formalism and codes to tackle the complete calculation.

The milestones for the review period as described in the Year-2 Continuation and Progress Report are in part different from the Schedule and Milestones for FY2013 (Year-3) described in the original research plan given in the grant proposal, and consist in:

- Implementation of the *NNN* force in the (*A*-1,1) + *A* no-core shell model with continuum:
  - Derivation and coding of the *NNN*-force couplings between nucleon-nucleus (*A*-1,1) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system;
  - Applications to nucleon-nucleus scattering with SRG-evolved *NN*+*NNN* chiral EFT potentials;
- Implementation of the (*A*-2,2) + *A* no-core shell model with continuum:
  - Derivation and coding of the overlap and of the *NN*- and *NNN*-force couplings between deuterium-nucleus (*A*-2,2) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system;
  - Applications to *d*-^{4}He scattering, *d*(^{3}H,*n*)^{4}He and *d*(^{3}He,*p*)^{4}He reactions, and possibly *n*-*n*-^{4}He scattering;
- Implementation of the coupled (*A*-3,3) + (*A*-2,1,1) NCSM/RGM:
  - Derivation and coding of the overlap matrix element and *NN*-force couplings between ^{3}He(^{3}H)-nucleus and nucleon-nucleon-nucleus NCSM/RGM bases;
  - *Ab initio* calculation of the overlap and Hamiltonian kernels between ^{3}H+^{3}H and ^{4}He+*n*+*n* NCSM/RGM bases using SRG-evolved *NN* chiral EFT potentials.
- Operator evolution for *ab initio* nuclear theory
  - SRG evolution of external operators in three-body space and application to the calculations of transition matrix elements in the A=4 system.

The last bullet, not present in the original research plan, was achieved in collaborations with Ph.D. Micah Schuster from California State University San Diego, who was hired and supported by this project as a Summer Student from May 20 to August 16, 2013.

Description of Accomplishments for the Review Period

Implementation of the NNN force in the (A-1,1) + A no-core shell model with continuum

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: P. Navrátil (TRIUMF)

The NCSM/RGM approach, based on expansions over fully-antisymmetric (A-a,a) binary-cluster states in the spirit of the RGM, in which each cluster of nucleons is described within the *ab initio* NCSM, has been successfully applied to a wide variety of binary processes,[2,3,4] starting from high-precision *NN* interactions. Extension of the approach to include the *NNN* force and the treatment of three-cluster dynamics are being developed as part of this project and showing promising results.[6,7] At the same time, these studies have highlighted practical limitations of the approach mainly related to a non-entirely efficient convergence behavior at short-to-medium distances. Here, to make up for missing *A*-body (composite-system) correlations, one has to introduce numerous excited or pseudo-excited states of the target and/or projectile nucleus. As an example, the description of the low-energy ^{7}Be(p,γ)^{8}B capture required taking into account the lowest five eigenstates of ^{7}Be,[3] and a much larger number of excited pseudostates is essential to address the virtual breakup of weakly-bound projectiles such as deuterium, ^{3}H, or ^{3}He, even at energies much below the breakup threshold.[2,4,8] This in turn results in a dramatic increase of complexity of the calculations as a large number of channels are coupled. The inclusion of the *NNN* force, which dramatically increases the computational effort required to calculate each term of the Hamiltonian kernel, exacerbates the situation even further. At the same time, the treatment of three-cluster dynamics, which in itself generates a large number of coupled channels, can quickly become computationally unfeasible if several excitations of the target have to be taken into account.

A more efficient approach to nuclear bound and continuum states is the no-core shell model with continuum (NCSMC).[9] Here one works in an extended model space that, in addition to the continuous binary-cluster (A-a,a) NCSM/RGM states, encompasses also square-integrable NCSM eigenstates of the A-nucleon system. Such eigenstates introduce in the trial wave function short- and medium-range A-nucleon correlations, significantly decreasing the need for excited states of the clusters in the NCSM/RGM sector of the basis. At the same time, the NCSM/RGM cluster states provide an effective description of the tail of the wave function, and make the theory able to handle the scattering physics of the system.

The development of the NCSMC is also very cost effective, if one considers that the NCSM/RGM component of it, which is the most complicated one, is well underway. The Hamiltonian and overlap couplings between NCSM/RGM (A-a,a) cluster states and NCSM A-nucleon eigenstates are the only new (and simpler to implement) elements of the approach.

The NCSMC overlap and Hamiltonian couplings for the case in which the binary-cluster portion of the basis is given by a single-nucleon projectile in relative motion with respect to a (A-1)-nucleon target were constructed considering only the *NN* component of the interaction between nucleons during the past reporting periods and were used to describe of the low-lying resonances of the exotic ^{7}He nucleus, using an SRG-evolved chiral EFT *NN* potential as detailed in Ref. [9]. The results obtained showed an impressive improvement in the convergence rate of the calculation.

During this review period we have completed that effort by including into the formalism the *NNN*-force. This required taking into consideration the additional interaction coupling between nucleon-nucleus (*A*-1,1) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system schematized in Fig. 1. This new coupling has been derived and implemented into our codes both using the standard factorization into terms depending on transition densities and by a direct application of the relevant creation and annihilation operators on the target and compound eigenvectors (more for details we refer the interested reader to Ref. [6]). The first approach is the most efficient when dealing with a total of four nucleons or less, while the second approach is best suited for larger mass systems. These two independent implementations have been verified by performing a benchmark calculation of nucleon-^{3}H scattering in small model spaces.

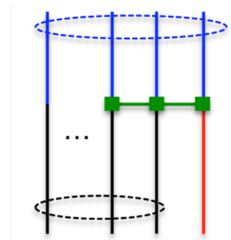

Figure 1. Diagrammatic representation of the matrix elements entering the calculation of the *NNN*-force NCSMC coupling for single nucleon projectiles. The groups of circled lines represent the (*A*−1)-nucleon target and A-nucleon eigenstates. Bottom and upper part of the diagram represent initial and final states, respectively.

These new computational tools were then used to perform large-scale NCSMC calculations of nucleon-^{4}He scattering including both SRG-induced and chiral *NNN* forces. This resulted in an impressive gain in the convergence rate and overall accuracy of our calculations, as evident when comparing the ^{4}He(*n*,*n*)^{4}He scattering phase shifts of Figs. 2a and 2b. The various curves represent results obtained with the chiral *NN*+*NNN* force as a function of the number of excited states of the ^{4}He included in the calculations. While in Fig. 2a, where the adopted model space is spanned only by *n*+^{4}He binary-cluster states,[6] the convergence pattern is quite slow and arguably not fully complete, the calculations of Fig. 2b, further including the first eight NCSM

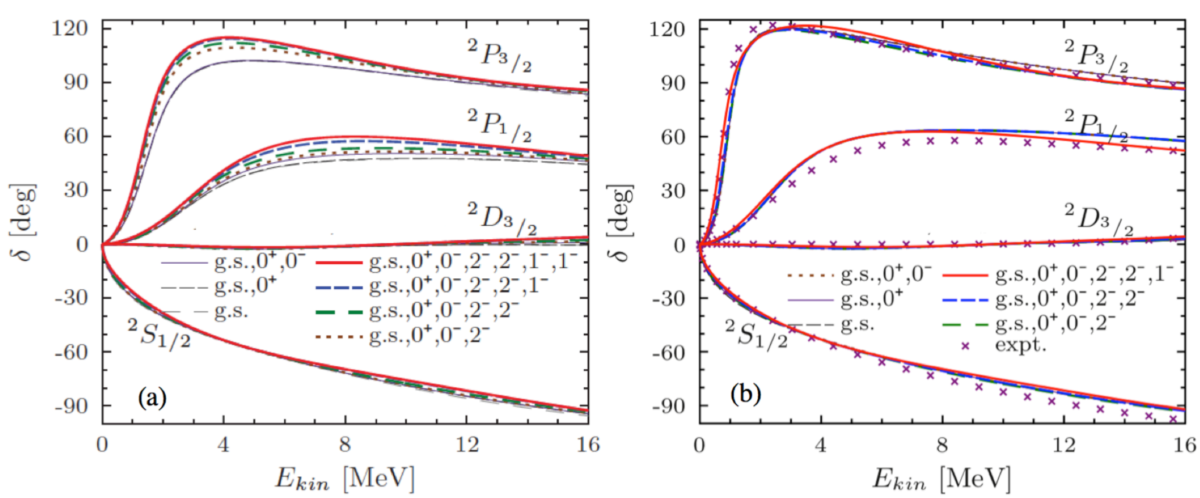

Figure 2 Scattering phase shifts for the ^{4}He(*n*,*n*)^{4}He reaction obtained using the SRG-evolved N^{3}LO *NN* + N^{2}LO *NNN* interaction with λ = 2.0 fm^{-1}, by (a) working within a *n*+^{4}He NCSM/RGM binary-cluster basis as in Ref. [6], and (b) further including the first eight NCSM eigenstates of ^{5}He. The calculations of panel (b) are also compared to experiment (crosses).

eigenstates of ^{5}He, are all but independent of the excitations of the ^{4}He nucleus and hence fully converged. At the same time, the NCSMC accurate results of Fig. 2b make use, and would have not been possible without, the NCSM/RGM groundwork of Fig. 2a which was initiated and performed under this project and has been now published in Ref. [6].

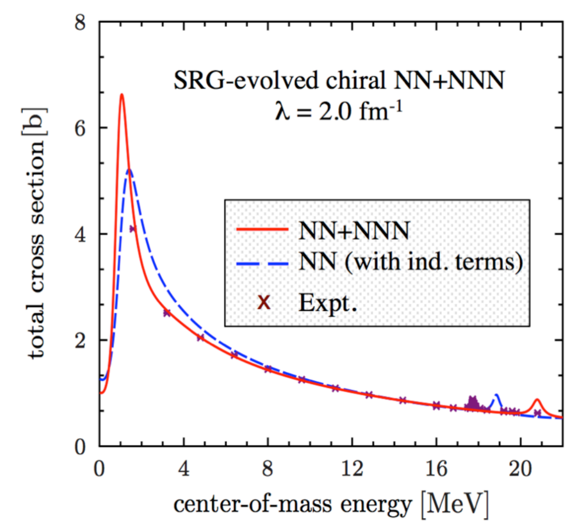

Figure 3 Calculated ^{4}He(n,n)^{4}He total cross section obtained within the *ab initio* NCSMC with (red solid line) and without (blue dashed line) *NNN* force compared to experimental data (crosses). See also caption of Figs. 2.

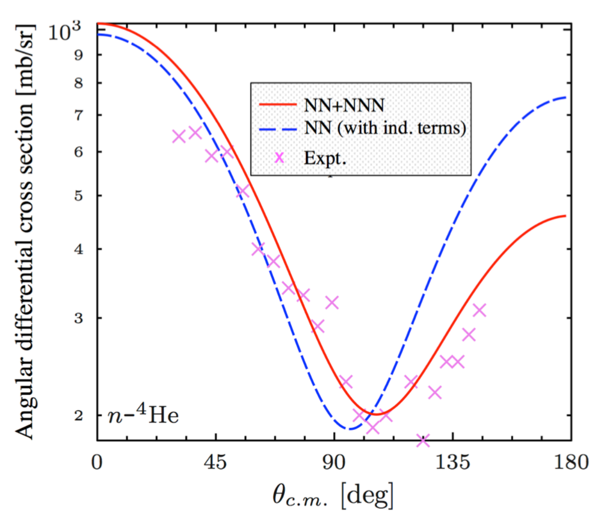

Figure 4 Calculated ^{4}He(n,n)^{4}He angular cross section for 1.79 MeV neutron incident energy obtained within the NCSMC with (red solid line) and without (blue dashed line) *NNN* force compared to experiment (crosses). See also caption of Fig. 2.

As shown in Fig. 2b, our neutron-^{4}He NCSMC calculations based on SRG-evolved *NN*+*NNN* forces from chiral effective field theory are in excellent agreement with experiment. Figure 3 and 4 further show that the inclusion of the *NNN* force (red curves) is essential to achieve such an agreement with experiment (crosses), particularly at low energies. The results obtained with the *NN* force alone (dashed blue lines) fail to describe the peak of the ^{4}He(n,n)^{4}He total cross section, shown in Fig. 3, as well as the minimum and overall shape of the angular cross section for 1.79 MeV neutron incident energy, shown in Fig. 4.

A manuscript describing (among other results) our study of neutron- and proton-^{4}He scattering with SRG-evolved *NN*+*NNN* chiral EFT potentials is in preparation and should be ready for submission by the end of the present reporting period or soon after, contingent the continuous availability of high-performance computing resources required to complete all necessary simulations (see item 13 of "Publications").

Implementation of the (A-2,2) + A no-core shell model with continuum

Personnel involved: G. Hupin (postdoc) and S. Quaglioni

Collaborators: P. Navrátil (TRIUMF)

During this review period we also initiated a systematic development of the NCSMC approach to treat binary-cluster states with composite projectiles, starting with the deuterium nucleus. In particular, we derived and implemented into our codes the overlap, the *NN*-, and *NNN*-force couplings between deuterium-nucleus (*A*-2,2) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system, respectively described by diagrams (a), (b) and diagrams (c) and (d) of Fig. 5. Different from the single-nucleon projectile case of Fig. 1, here the

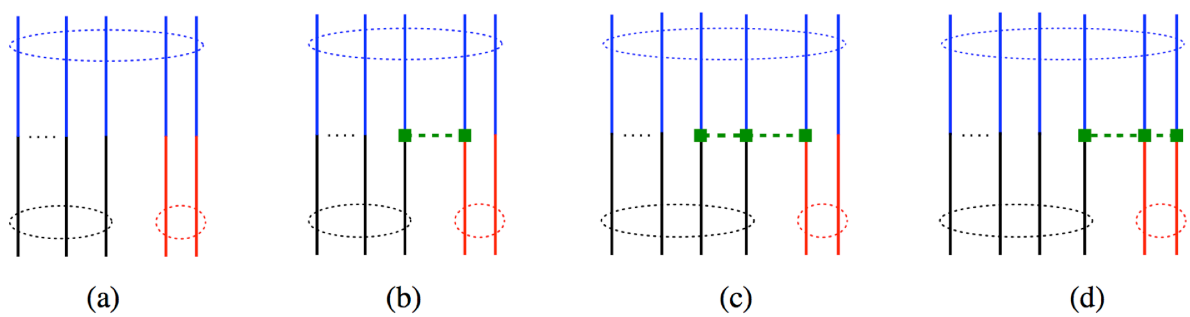

Figure 5. Diagrammatic representation of the matrix elements entering the calculation of (a) the overlap, (b) *NN*-force, and (c) and (d) *NNN*-force NCSMC couplings for a deuterium projectile. The groups of circled lines represent the 2-nucleon projectile, the (A−2)-nucleon target and the A-nucleon eigenstates. Bottom and upper part of the diagrams represent initial and final states, respectively.

inclusion of the *NNN* force involves the calculation of two coupling terms: diagram (c) coming from the interactions of two target nucleons with one of the projectile nucleons, and diagram (d) in which the *NNN* force is among the two nucleons inside the deuterium projectile and one of the target nucleons. All four NCSMC couplings have been derived and successfully implemented into our codes. Once again, we followed two parallel and independent strategies: a direct application of the relevant creation and annihilation operators on the NCSM eigenvectors, as well as a factorization into density-dependent terms. The two approaches have been then verified by performing a benchmark of d-^{2}H scattering in small model spaces.

If the NCSMC is very advantageous for nucleon-nucleus scattering, it is essential when describing collisions with composite projectiles such as the deuterium. There the large number of coupled channels required to address the virtual breakup of the projectile makes it computationally very hard or simply impossible to include in the calculation excited states of the target. This in turn results into an incomplete description of the scattering process at low energies as exemplified by the ^{4}He(d,d)^{4}He angular differential cross section for 2.935 MeV deuterium incident energy, shown in Fig. 6. Here the blue dashed line, obtained within a model space spanned only by d+^{4}He(g.s.) binary-cluster states, is clearly at odds with the available experimental data despite the inclusion into the calculation of up to six pseudo excited states of the deuterium projectile in three different channels ($^3S_1$-$^3D_1$, $^3D_2$, and $^3D_3$-$^3G_3$). The further inclusion of the first six eigenstates of the ^{6}Li nucleus, which is the compound system for this reaction, radically improves the agreement with experiment (red solid line).

In general we find that the inclusion of ^{6}Li eigenstates not only dramatically improves the description of the scattering process at lower energies, but also substantially reduces the influence of the excited pseudostates of the deuterium. These, however, have still to be taken into account to address the virtual breakup of the weakly bound projectile.

The substantial importance of the *NNN* force emerged from the study of neutron-^{4}He scattering is confirmed and further emphasized by the ^{4}He(d,d)^{4}He phase shifts of Fig. 7. Here, the *NNN* force (red solid lines) is responsible for shifting the centroid of the low-lying $^3D_3$ resonance of about 1 MeV closer to experiment, doubling the splitting between this and the $^3D_1$ and $^3D_2$ phase shifts with respect to the results obtained with only the *NN* interaction (dashed blue lines). The agreement with the experimental phase shifts also improves in the $^3S_1$ partial wave, when the *NNN* interaction is taken into account. In this channel we also find one bound state, the ground state of ^{6}Li, with a binding energy of 1.79 MeV with respect to the d+^{4}He breakup threshold, in fairly good agreement with the experimental value of 1.4743 MeV. While these results are extremely promising, we expect that calculations in a larger harmonic oscillator model space containing up to N_{max} = 11 quanta above the minimum energy configuration will improve agreemnt with experiment even further.

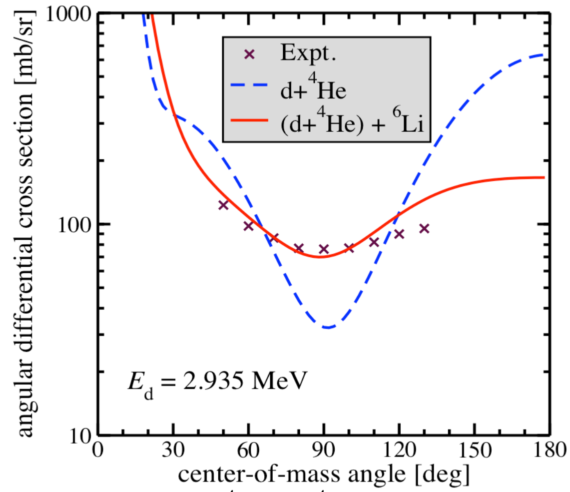

Figure 6 Calculated ^{4}He(d,d)^{4}He angular differential cross section for 2.935 MeV deuterium incident energy obtained with (red solid line) and without (blue dashed line) inclusion of ^{6}Li eigenstates. This example was obtained using only the *NN* component of the SRG-evolved N^{3}LO *NN* interaction with λ = 2.0 fm^{-1} an HO space of size N_{max}=9 and frequency $\hbar\Omega$=20 MeV.

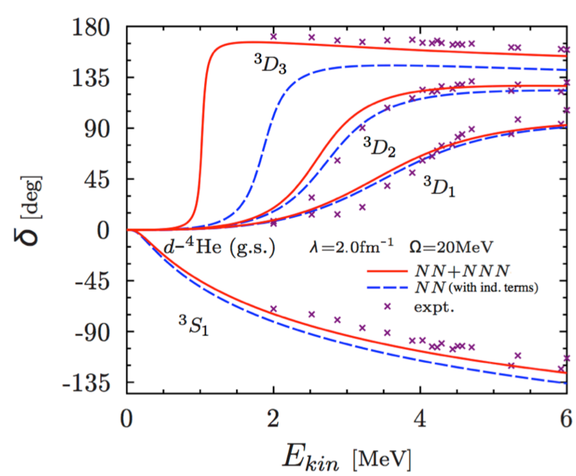

Figure 7 Calculated ^{4}He(d,d)^{4}He scattering phase shifts obtained within the NCSMC with (red solid line) and without (blue dashed line) *NNN* force compared to experiment (crosses). See also caption of Fig. 6.

Once again, the present NCSMC results for deuterium scattering on ^{4}He make use, and would have not been possible without, the NCSM/RGM groundwork of Years 1 and 2 of this project. A manuscript reporting on these and other results is in preparation and should be ready for submission by the end of the present reporting period or soon after, contingent the continuous availability of high-performance computing resources required to complete all necessary simulations (see item 13 of "Publications").

Finally, using the developed NCSMC formalism and codes for the description of nucleon- and deuterium-nucleus scattering states we are on track to deliver initial results for the $d(^3\text{H},n)^4\text{He}$ and $d(^3\text{He},p)^4\text{He}$ fusion reactions with chiral *NN*+*NNN* forces. However, we anticipate that this study will be completed during the next reporting period.

Implementation of the coupled (A-3,3) + (A-2,1,1) NCSM/RGM

Personnel involved: S. Quaglioni

For reactions involving a ^{3}H(^{3}He)-nucleus entrance and nucleon-nucleon-nucleus three-cluster exit channels [*e.g.*, $^3\text{H}(^3\text{H},2n)^4\text{He}$] or *vice versa*, and, more in general, whenever both ^{3}H(^{3}He)-nucleus and nucleon-nucleon-nucleus channel basis states are used in the RGM model space, one has to address the contributions to the integration kernels coming from the off-diagonal matrix elements between the two mass partitions: (*A*-3,3) and (*A*-2,1,1). For the norm kernel we have identified three terms, schematically represented by the diagrams of Fig. 8: (a) the overlap between the initial (A−3,3) binary-cluster and final (A-2,1,1) three-cluster state; (b) a one-nucleon exchange term; and, (c) a two-nucleon exchange term. In the next few months, we plan to derive and implement into our NCSM/RGM codes the algebraic expressions for these terms as well as for those entering the Hamiltonian kernel with a *NN* interaction.

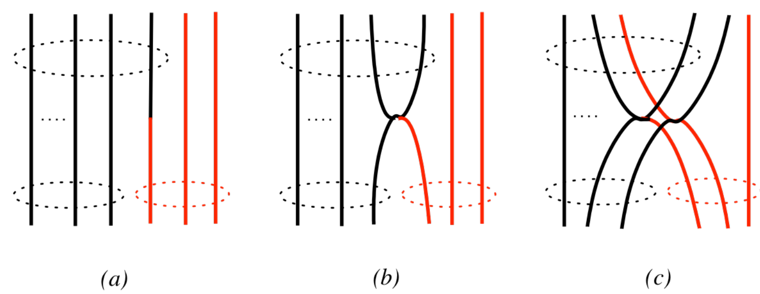

Figure 8. Diagrammatic representation of: (a) "overlap", (b) "one-nucleon-exchange", and (c) "two-nucleon-exchange" components of the norm kernel for an (A−3, 3) mass partition in the initial state and an (A−3,1,1) mass partition in the final state. The groups of circled lines represent the (A−3)-, (A−2)-, and three-nucleon clusters. Bottom and upper part of the diagram represent initial and final states, respectively.

First investigation of the ^{4}He+n+n continuum within an ab initio framework

Personnel involved: S. Quaglioni

Collaborators: C. Romero Redondo and P. Navrátil (TRIUMF)

A rigorous description of nuclei for which the lowest threshold for particle decay is of the three-body nature, such as ^{6}He or ^{11}Li, requires the treatment of three clusters in the continuum of energy. The same is true of nuclear reactions characterized by three-body final states, such as the $^3\text{He}(^3\text{He},2p)^4\text{He}$ solar rate or the $^3\text{H}(^3\text{H}, 2n)^4\text{He}$ process used in diagnostics of modern fusion experiments. In the previous reporting periods we had developed the NCSM/RGM formalism and codes to calculate bound and continuum states of three-cluster systems formed by two separate nucleons in relative motion with respect to a nucleus of mass number *A*-2, and obtained the first *ab initio* description of the ^{6}He ground state within a ^{4}He(g.s.)+*n*+*n* three-cluster basis. This work has now been published in the journal article of Ref. [7].

In the present reporting period we have completed the first study of the low-lying continuum of the ^{6}He nucleus within an ab initio framework that encompasses the ^{4}He+n+n three-cluster dynamics characterizing its lowest decay channel. In particular, we have explored in detail the convergence of our calculations with respect to the various parameters characterizing our three-cluster model space. All calculations have been performed with the SRG-evolved N^{3}LO *NN* interaction with λ = 1.5 fm^{-1} and an $\hbar\Omega$=14 MeV harmonic oscillator frequency. As an example, Fig. 9 shows the dependence of calculated ^{4}He+*n*+*n* phase shifts for four different channels of angular momentum and parity with respect to the maximum number of harmonic oscillator excitations above the minimum energy configuration $N_{\max}$ used to build the NCSM/RGM channel states. A fairly good convergence is reached at $N_{\max}$ = 13.

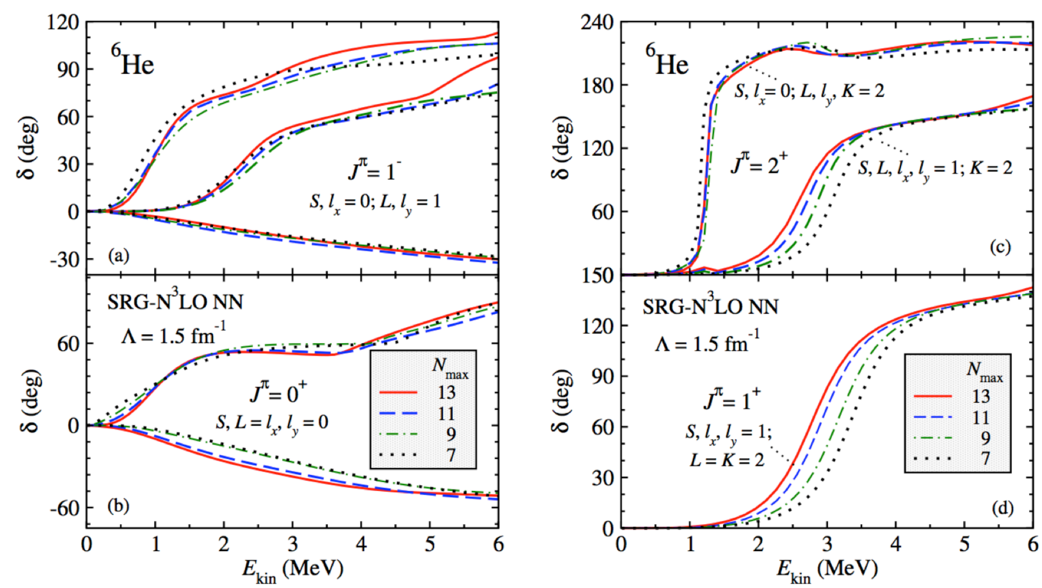

Figure 9 Convergence behavior of calculated ^{4}He+*n*+*n* (a) $J^\pi = 1^-$ and (b) 0^+ eigenphase shifts at $K_{\max}$ = 19 and 28, respectively, and (c) 2^+ and (d) 1^+ diagonal phase shifts with respect to the size $N_{\max}$ of the NCSM/RGM model space. For these calculations we used a matching radius of a = 30 fm and an extended harmonic oscillator model space of $N_{\rm ext}$ = 70.

Another important parameter is the hyperradius a used to match the logarithmic derivative of the three-cluster wave function in the interior and exterior regions and find the elements of the scattering matrix (for more details, we refer the interested reader to Ref. [7]). We found that in our approach the value of a needed to reach the asymptotic conditions in which all three fragments are far apart from each other is correlated with the parameter $N_{\rm ext}$. This is the size of an extended harmonic oscillator basis used to represent a Dirac's δ function in the distance between the ^{4}He and the two interacting neutrons. Larger $N_{\rm ext}$ values correspond to a larger range for this potential kernel, hence requiring a larger hyperradius in order to reach the external (interaction free) region. This is exemplified by the phase shifts of Fig. 10, where is shown how the same matching radius of $a = 30$ fm sufficient to obtain stable results for $N_{\rm ext}$ values up to 100 becomes too small for $N_{\rm ext} = 200$.

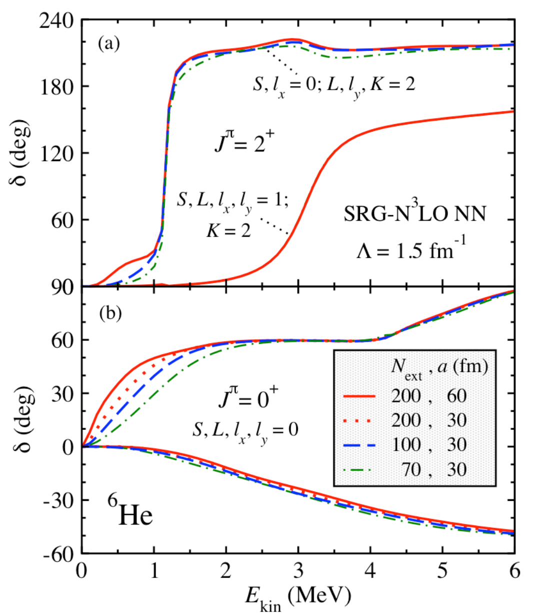

Figure 10 Dependence on the size of the extended HO model space $N_{\rm ext}$ used to describe the neutron-neutron interaction in the external region of calculated ^{4}He+n+n (a) $J^\pi = 2^+$ diagonal phase

We further found that the influence of $N_{\rm ext}$ and the need for larger values of a is confined to very low energies (below 1 MeV) and is most pronounced for attractive phase shifts in which the two neutrons are in s-wave relative motion. There the neutron-neutron interaction is larger and the wave function is more extended due to the Pauli exclusion principle. In particular, the value of $N_{\rm ext}$ has little or no influence on the position and width of the resonant phase shifts, as shown in Fig. 10 for the 2^+ phase shifts.

The positions and widths of our calculated resonances are compared to measurements performed at the SPIRAL facility (GANIL, France)[10] in Fig. 11. Except for an overall shift in energy, we can describe the first three positive-parity states in agreement with experiment. In particular, our theory can explain the existence of a second 2^+ resonance, which was observed for the first time at SPIRAL, and predicts new negative parity states not yet known experimentally. Based on these very promising results, we expect that the accuracy of our calculations and agreement with experiment will improve further in an extended NCSMC calculation including eigenstates of the compound ^{6}He nucleus and the *NNN* force. A manuscript reporting on these and other results is in preparation and should be ready for submission by the end of the present reporting period or soon after (see item 12 of "Publications").

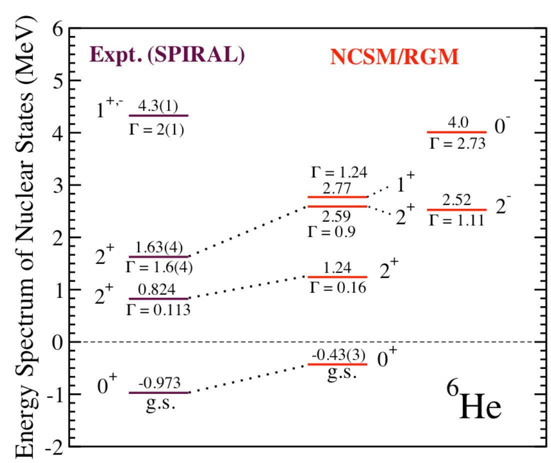

Figure 11 Calculated positive- and negative parity low-lying states of ^{6}He compared to the spectrum measured at the SPIRAL facility, GANIL.[10] Energy centroids and widths of the levels above the ^{4}He+n+n breakup threshold are extracted from the calculated resonant phase shifts.

Operator evolution for ab initio nuclear theory

Personnel involved: M. D. Schuster (Summer Ph.D. Student), S. Quaglioni

Collaborators: C. Johnson (SDSU), E. D. Jurgneson (LLNL), and P. Navrátil (TRIUMF)

Success in the ab initio description of light-nucleus reactions with the NCSM/RGM and NCSMC approaches has been made possible in part by the development of modern effective interaction theory, where the size of the model space required for an accurate solution of the many-body problem is substantially reduced by means of unitary transformations of the nuclear Hamiltonian. In particular, in our calculations we use similarity-renormalization group or SRG evolved two- and three-body forces. However, caution has to be taken when these interactions are used to describe, e.g., perturbation-induced reactions, where the cross section is a continuous observable depending on matrix elements of external transition operators between initial and final states. Indeed, for a fully consistent calculation the same unitary transformation applied to the Hamiltonian should be applied to any external operator. As for the Hamiltonian, this generates induced many-body terms.

Working in a translationally invariant harmonic oscillator basis for the two- and three-nucleon systems, we implemented the renormalization of external operators up to the three-body level in the framework of the SRG and studied for the first time the behavior of such renormalized three-body operators in systems with more than three nucleons, thus assessing the importance of higher-body terms. Figure 12 shows the results for (a) the root-mean-square (RMS) radius and (b) total strength of the dipole transition in ^{4}He. The trends of these results are similar because the operators are closely related [11]. When using the bare operator, the observable has significant λ dependence at small values. However, when evolved in the two- and then in the three-body space, independence is all but restored. The transformation is not completely unitary due to the SRG induced four-body terms that we do not include. This causes a slight increase in the calculated observables at smaller λ values, as emphasized for the RMS radius, for which we show also the expectation value obtained with the bare *NN*+*NNN* Hamiltonian and bare operator (dotted line). This bare result can be also recovered at large lambda values, where the induced terms affecting the operator become increasingly smaller. The trade off, however, is a much slower convergence rate, which would require prohibitively large model space sizes for heavier-mass systems. There, λ is typically chosen between 1.8 and 2.0 fm^{-1}, where one can speed up the convergence while keeping to a

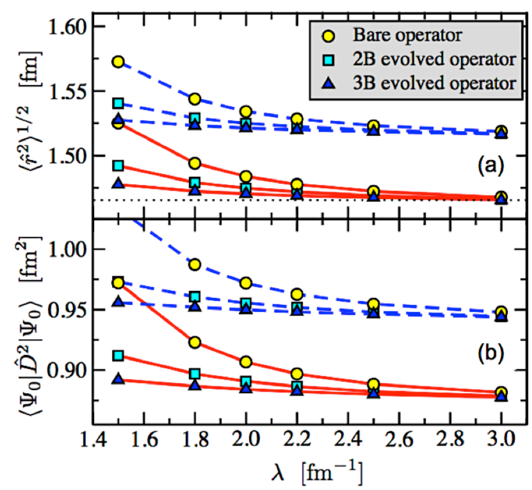

Figure 12 Calculated (a) RMS radius and (b) total dipole strength of ^{4}He as a function of SRG evolution parameter, λ. Shown are results obtained with (red solid line) and without (blue dashed line) *NNN* force, and with three levels of operator evolution: bare operator (circles), operator evolved in the two-body space (squares), and operator evolved in the three-body space (triangles). The dotted line is the RMS radius with bare Hamiltonian and bare operator.

minimum the effect of beyond-three-body induced forces.

This work sets the stage for high-precision calculations of observables at the intersection between nuclear physics and other fields, such as the polarization of a nucleus, important in Lamb shift measurements of nuclear radii, radiative capture reactions crucial to understanding the neutrino signature of our sun, or radiative cross sections used for plasma diagnostics in fusion experiments. A manuscript reporting on this study has been submitted to Physical Review Letters.[12]

Opportunities for Training and Development

Personnel involved: M. Schuster, S. Quaglioni

Collaborators: C. Johnson (SDSU)

During this review period the project "Solving the Long-Standing Problem of Low-Energy Nuclear Reactions at the Highest Microscopic Level" will provide the following opportunities for training and developments of graduate students.

Returning Summer Student Micah Schuster

Micah Schuster, a Ph.D. student at San Diego State University, should be hired and supported by this project as a Summer Student for about 10 weeks between May and August 2014. Under the supervision of Dr. Quaglioni, Mr. Schuster will continue studying the consistency of the similarity renormalization group approach for perturbation-induced reactions, where the cross section is a continuous observable depending on matrix elements of external transition operators between initial and final states. In particular, during Year 3 of the project Mr. Schuster will extend the use of three-body evolved external operators to heavier systems (e.g. A = 5 - 12), where it is computationally more advantageous to work with single-particle Slater determinant basis states. This can be accomplished by transforming the present translationally invariant three-body operators into matrix elements over Slater determinant three-nucleon basis states, similarly to what has been done for the *NNN* force.

This work benefits this DOE/SC/NP project by enhancing *ab initio* efforts to describe light-ion fusion reactions relevant for nuclear astrophysics and Laboratory programs, particularly radiative captures and bremsstrahlung processes involving transition matrix elements of external electromagnetic operators.

Dissemination

Publications

1. **"**Ab initio many-body calculations of nucleon-^{4}He scattering with three-nucleon forces", G. Hupin, J. Langhammer, P. Navrátil, S.Quaglioni, A. Calci, and R. Roth, Physical Review C **88,** 054622 (2013).
2. "Three-cluster dynamics within an ab initio framework", S. Quaglioni, C. Romero-Redondo and P. Navrátil, Physical Review C **88**, 034320 (2013).
3. "Unified ab initio approach to bound and unbound states: no-core shell model with continuum and its application to ^{7}He", S. Baroni, P. Navrátil and S. Quaglioni, Physical Review C **87**, 034326.
4. "Computational nuclear quantum many-body problem: The UNEDF project", S. Bogner et al., Computer Physics Communications **184**, 2235 (2013).
5. "Ab initio calculations in three-body cluster systems", C. Romero-Redondo, P. Navrátil, and S. Quaglioni, AIP Conference Proceedings **1541**, 156 (2013).
6. "T-T neutron spectrum from inertial confinement implosions", A. D. Bacher et al., Few-Body Syst. **54**, 1599 (2013).
7. "Progress on Light-Ion Fusion Reactions with Three-Nucleon Forces", G. Hupin, S. Quaglioni, J. Langhammer, P. Navrátil, A. Calci, R. Roth, Few-Body Systems (2014) in print, DOI 10.1007/s00601-013-0800-4, arXiv:1401.0365.
8. "Operator evolution for ab initio nuclear theory", M. D. Schuster, S. Quaglioni, C. W. Johnson, E. D. Jurgenson, and P. Navrátil, submitted to Physical Review Letters, arXiv:1402.7106.
9. "Precision measurement of the electromagnetic dipole strengths in ^{11}Be", E. Kwan et al., submitted to Physics Letters B.
10. "Ab initio NCSM/RGM for three-body cluster systems and application to ^{4}He+n+n", C. Romero-Redondo, P. Navrátil, S. Quaglioni, and G. Hupin, submitted to Few-Body Systems, arXiv:1311.4595.
11. "Ab initio many-body calculations of the ^{4}He photo-absorption cross section", M. D. Schuster, S. Quaglioni, C. W. Johnson et al., arXiv:1304.5491.

Papers in Preparation

12. **"**^{4}He+n+n continuum within an ab initio framework", C. Romero-Redondo, S. Quaglioni, P. Navrátil, and G. Hupin, to be submitted to Physical Review Letters.
13. "Five- and six-nucleon scattering from chiral two- and three-body Hamiltonians", G. Hupin, P. Navrátil, and S. Quaglioni, to be submitted to Physical Review Letters.

Invited Talks (most recent first)

1. "Toward a fundamental understanding of nuclear fusion", by S. Quaglioni, Lawrence Livermore National Security/Los Alamos National Security Science & Technology Joint Committee Meeting of the Board of Governors, Livermore, CA, January 28, 2014.
2. "From nucleons, to nuclei, to fusion reactions", by S. Quaglioni, West Coast Conference for Undergraduate Women in Physics – 2014, UC Berkeley, January 19, 2014.
3. "Toward a Realistic Description of Light-ion Fusion Reactions for Astrophysics", by G. Hupin, IHPC/CNRS, Strasbourg, France, September 17, 2013.
4. "Toward Realistic Description of Low-energy Fusion of Light Ions for Astrophysics", by G. Hupin, University of Notre Dame, Notre Dame, Indiana, April 8, 2013.

Contributed Talks

1. "Ab initio nuclear theory including the continuum", by S. Quaglioni, TRIUMF Theory Workshop "Nuclear Structure and Reactions: Experimental and Ab Initio Theoretical Perspectives", TRIUMF, Vancouver, BC, Canada, February 18 - 21, 2014.
2. "Five- and six-nucleon scattering from QCD-based interaction", by G. Hupin, TRIUMF Theory Workshop "Nuclear Structure and Reactions: Experimental and Ab Initio Theoretical Perspectives", TRIUMF, Vancouver, BC, Canada, February 18 - 21, 2014.
3. "Recent progress towards ab initio calculations of light-nuclei reactions", by G. Hupin, EMMI program on "Halo Physics at the Neutron Drip Line", GSI Darmstadt, Germany, February 3 – 14, 2014.
4. "Progress on Light-Ion Fusion Reactions with Three-Nucleon Forces", by G. Hupin, 22nd European conference on few-body problems in physics, Cracow, Poland, September 9 - 13, 2013.
5. "Toward realistic calculations of light-ion fusion reactions", By G. Hupin, Canadian Association of Physics Congress, Montreal, Canada, May 27 – 31, 2013.

Additional Information

Plans for the Next Budget Period

To achieve the major goals and objectives of our research activity as described in our original research plan, we have found necessary to modify (in part) the plans for the next budget period compared to those initially proposed in Schedule and Milestones for FY2014 (Year 4) given in the grant proposal. The modified plans for the next budget period consist in:

- Applications of recently developed NCSMC formalism and codes for the description of nucleon- and deuteron-nucleus continua with *NN*+*NNN* forces:
  - First *ab initio* calculation of the ^{3}H(d,n)^{4}He and ^{3}He(d,p)^{4}He fusion reactions within the (A-1,1) + (A-2,2) + A no-core shell model with continuum using SRG-

evolved *NN+NNN* chiral EFT potentials;

- Applications of recently developed NCSM/RGM formalism and codes for the description of nucleon-nucleon-nucleus three-cluster dynamics with *NN* potentials:
  - Spectroscopy of ^{5}H within the ^{3}H+*n*+*n* NCSM/RGM basis using SRG-evolved *NN* chiral EFT potentials;
  - Spectroscopy of ^{11}Li within the ^{9}Li+*n*+*n* NCSM/RGM basis using SRG-evolved *NN* chiral EFT potentials;
- Implementation of the coupled (*A*-2,1,1) + *A* no-core shell model with continuum formalism and codes for the description of nucleon-nucleon-nucleus three-cluster dynamics with *NN+NNN* forces:
  - Derivation and coding of the *NN*- and *NNN*-force couplings between (*A*-2,1,1) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system;
  - Application to ^{4}He+*n*+*n* bound and continuum states using SRG-evolved *NN+NNN* chiral EFT potentials;
- Implementation of (A-3,3) + A no-core shell model with continuum
  - Derivation and coding of the *NN*- and *NNN*-force couplings between (*A*-3,3) NCSM/RGM channel states and NCSM *A*-body eigenstates of the composite system;
  - Application to ^{3}H(^{3}He)+^{4}He scattering and ^{7}Li(^{7}Be) spectroscopy;
- Development of framework for the solution of the scattering problem in the presence of a binary cluster entrance channel and three-cluster exit channel

Different from the original deliverables, we plan to apply the three-cluster NCSM/RGM approach to study the spectroscopy of ^{11}Li within the ^{9}Li + *n* + *n* basis using SRG-evolved *NN* chiral EFT potentials. This deliverable, originally planned for Year 2 of the project, had been delayed due to the challenge of computing three-body densities of the A = 9 target, an intermediate step previously required by the formalism. To resolve this issue, we have been pursuing a novel approach of calculating the NCSM/RGM projectile-target potentials by a direct application of the relevant creation and annihilation operators on the target eigenvectors rather than by factorization into density-dependent terms. These new computational tools should now allow us to address the spectroscopy of the ^{11}Li nucleus during Year 4.

At the same time, we will postpone the development of the three-cluster NCSM/RGM formalism for nucleon-deuteron-nucleus systems in favor of the implementation of the no-core shell model with continuum for the description of ^{3}H(^{3}He)-nucleus scattering. Given the computational challenges that we have encountered so far and those ahead of us, such extension of the NCSMC approach is a essential to achieve the major goals and objectives of our research activity, and will lead to an improved description of the ^{7}Li and ^{7}Be nuclei.

Impact

A successful completion of this project will result in improved accuracy of the ^{3}He(^{3}He,2p)^{4}He and ^{3}He(α,γ)^{7}Be reaction rates and consequently, in enhancement of the predictive capability of the standard solar model. In addition, we will study also the mirror reactions ^{3}H(^{3}H,2n)^{4}He and ^{3}H(α,γ)^{7}Li (a key reaction for the production of ^{7}Li in the standard big-bang nucleosynthesis), and the spectroscopy of the ^{6}He, ^{6}Be, and ^{11}Li nuclei.

Participants

Project Personnel

- S. Quaglioni, PI
- G. Hupin, Postdoctoral Researcher
- M. Schuster (SDSU), Summer Ph.D. Student

External Visitors

- Postdoctoral Researcher Carolina Romero-Redondo (TRIUMF) visited Dr. Quaglioni at LLNL, supported from her home institution, from the 9 to the 19 of December 2013.

Collaborators

These collaborators contributed to our project, but were not funded by this grant:

- Dr. P. Navrátil (TRIUMF)
- Postdoctoral Researcher Carolina Romero-Redondo (TRIUMF)
- Dr. R. Roth (TU Darmstadt)
- Ph.D. Student J. Langhammer (TU Darmstadt)
- Ph. D. Student A. Calci (TU Darmstadt)
- Dr. C. Johnson (SDSU)

Student Tracking Information

Student	Date Entered Grad. School	Date Joined Group	Degree Program	Date Degree Expected	Advisor
M. Schuster	Aug, 2007	May-Aug, 2014	Ph.D.	Fall 2014	C. Johnson

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